

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041423\
 Data File : BG057102.D
 Acq On : 14 Apr 2023 16:22
 Operator : CG/JU
 Sample : 02347-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20230337-COMP-15

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057102.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.436	316	323	330	rBV	89390	139843	13.16%	2.247%
2	5.917	398	405	414	rVB	393526	644769	60.66%	10.362%
3	7.539	673	681	689	rBV	411960	699960	65.85%	11.249%
4	8.402	822	828	835	rBB	69496	114764	10.80%	1.844%
5	9.583	1019	1029	1037	rBV	232085	419657	39.48%	6.744%
6	11.239	1303	1311	1319	rBV	88653	160059	15.06%	2.572%
7	13.642	1713	1720	1727	rBV	555991	842831	79.30%	13.545%
8	15.017	1947	1954	1961	rVB2	139374	219022	20.61%	3.520%
9	16.350	2175	2181	2191	rBV	75120	105324	9.91%	1.693%
10	16.497	2199	2206	2213	rBV	493861	762135	71.70%	12.248%
11	17.754	2412	2420	2426	rBV	173201	259547	24.42%	4.171%
12	18.588	2557	2562	2571	rBV2	45697	69240	6.51%	1.113%
13	19.840	2771	2775	2780	rBV6	10165	14980	1.41%	0.241%
14	20.321	2851	2857	2863	rBV	834507	1062901	100.00%	17.082%
15	20.586	2897	2902	2905	rBV3	9957	13645	1.28%	0.219%
16	21.097	2984	2989	2992	rBV2	13900	19206	1.81%	0.309%
17	21.631	3075	3080	3089	rVB2	38904	62267	5.86%	1.001%
18	22.072	3148	3155	3161	rBV	149931	266052	25.03%	4.276%
19	22.219	3175	3180	3187	rVB3	14051	23356	2.20%	0.375%
20	22.871	3288	3291	3297	rVB7	10448	17465	1.64%	0.281%
21	24.516	3565	3571	3576	rVB9	9169	19262	1.81%	0.310%
22	25.602	3744	3756	3769	rVB2	85693	272953	25.68%	4.387%
23	26.795	3957	3959	3966	rVB6	6926	13036	1.23%	0.210%

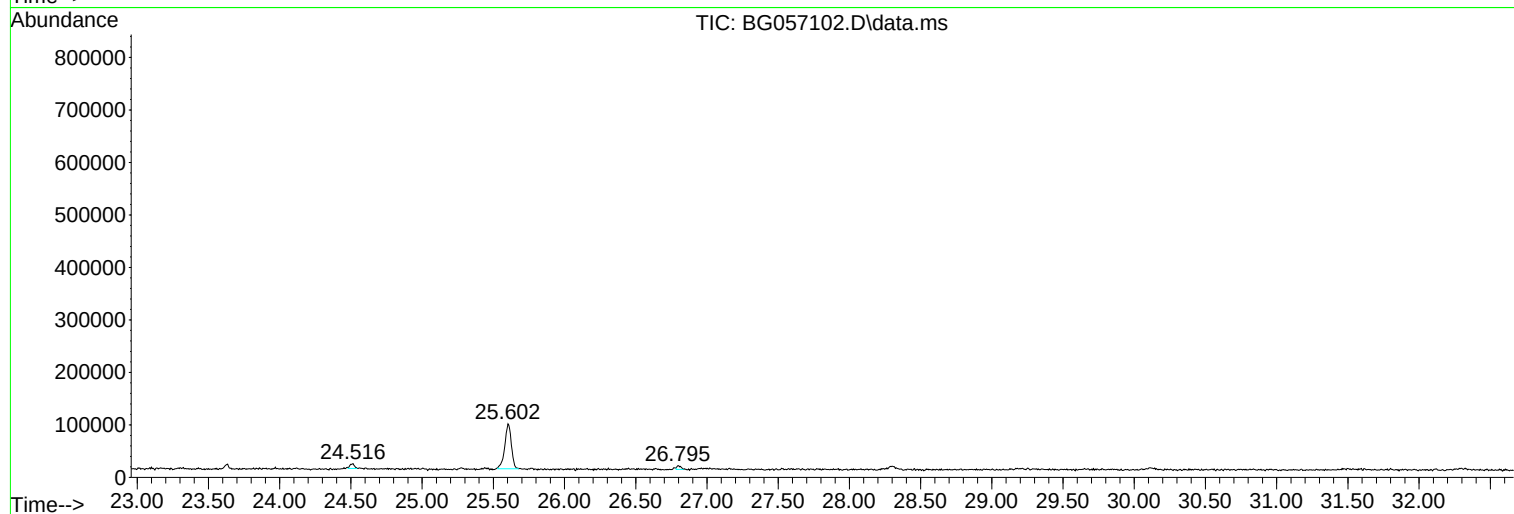
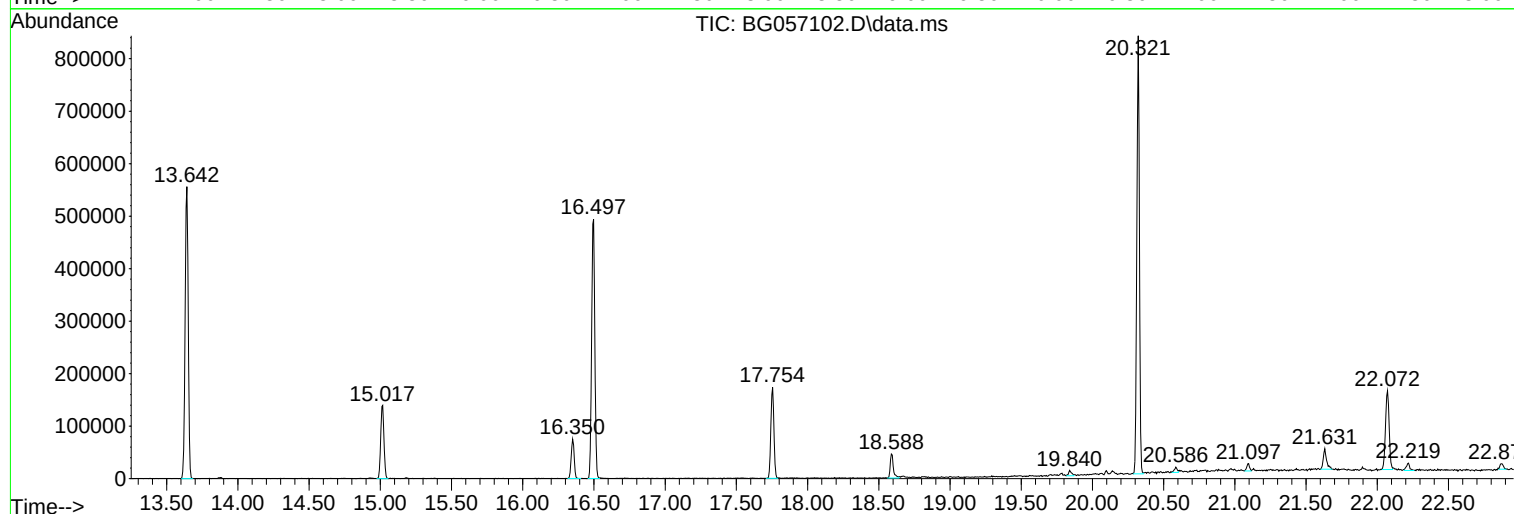
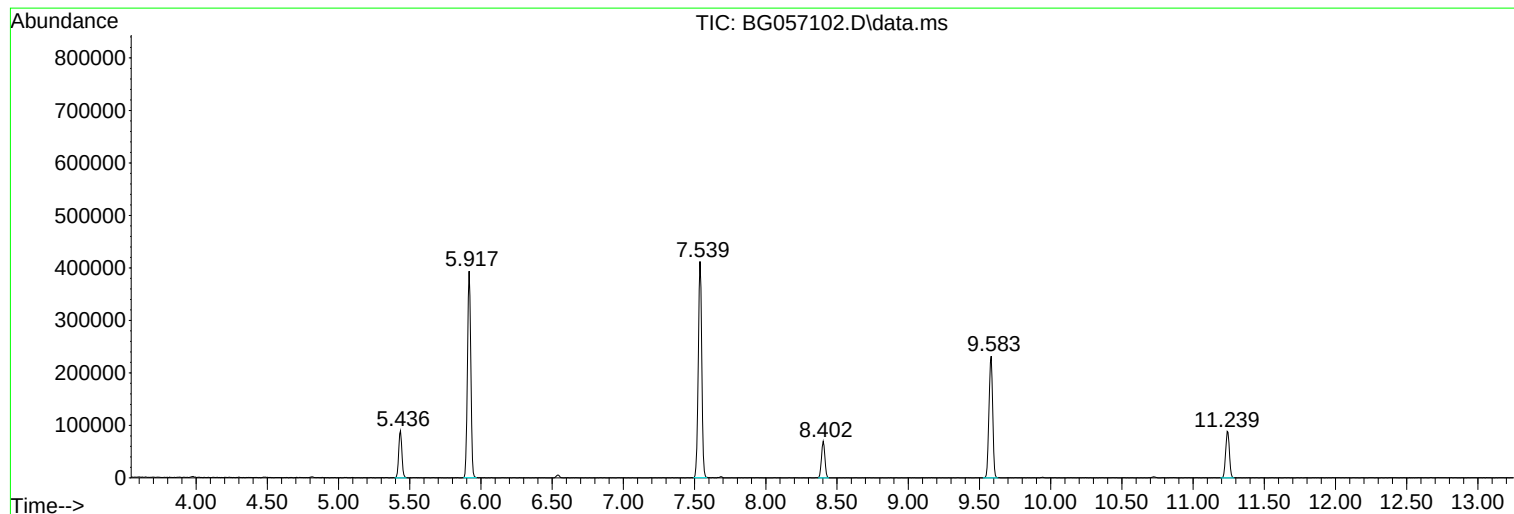
Sum of corrected areas: 6222274

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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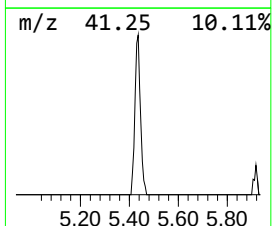
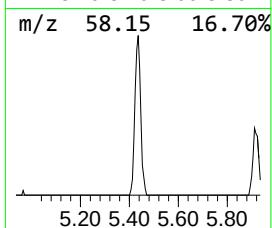
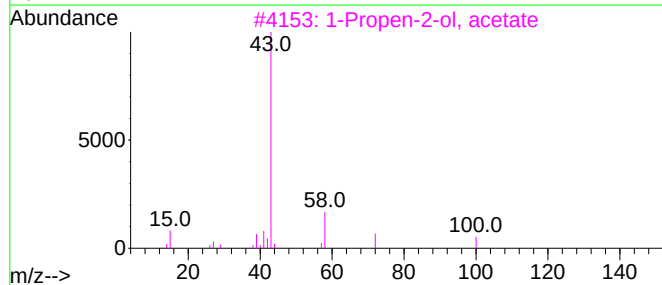
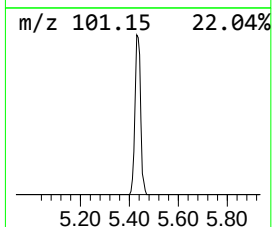
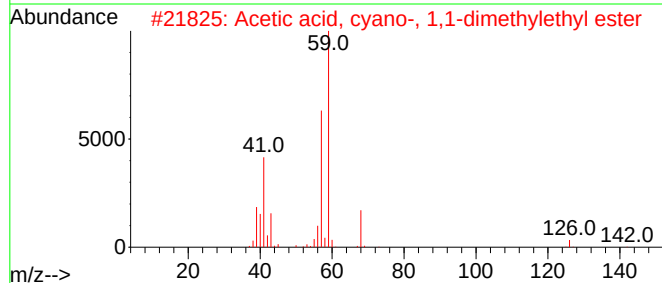
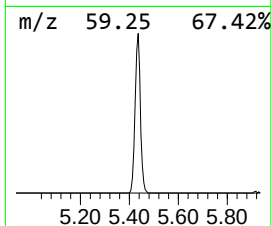
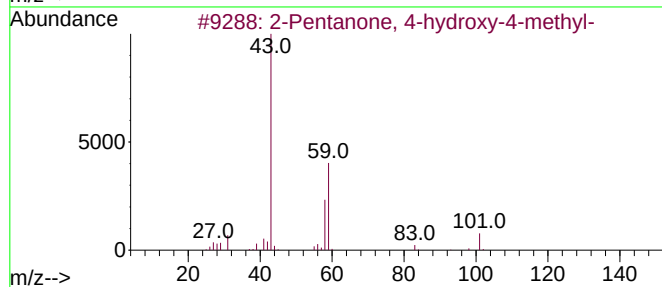
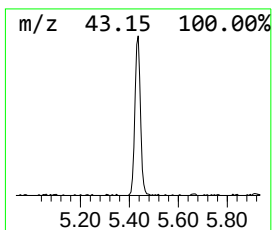
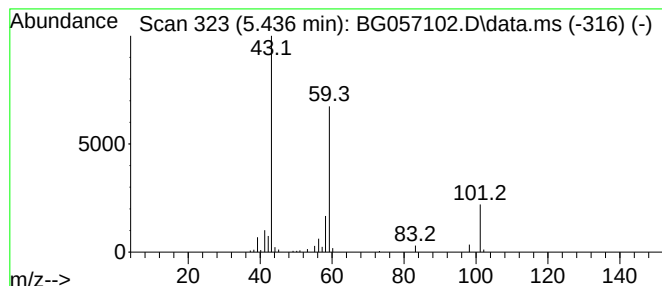
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.436	24.37 ng	139843	1,4-Dichlorobenzene-d4	8.402

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Acetone	58	C3H6O	000067-64-1	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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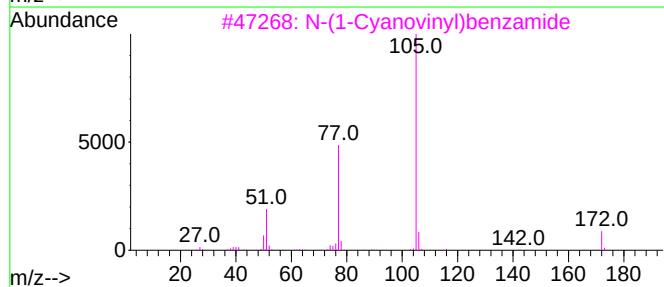
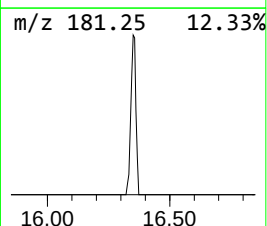
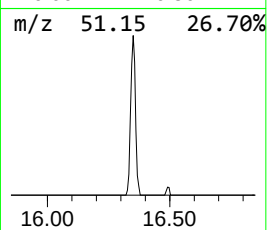
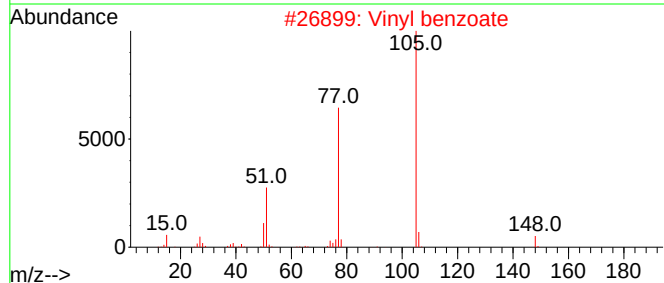
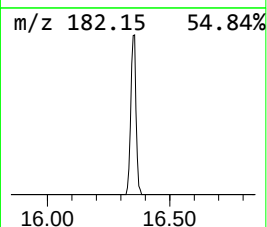
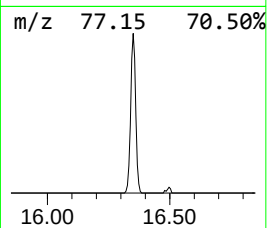
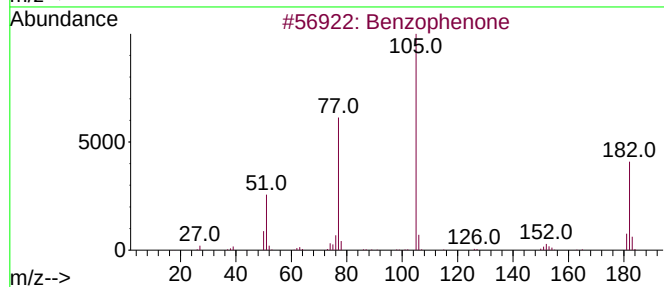
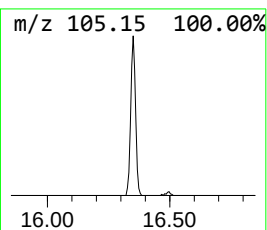
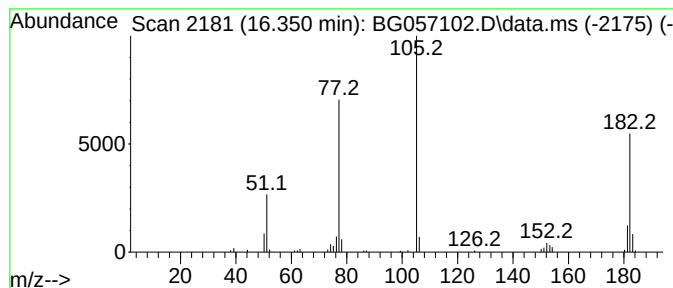
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.350	9.62 ng	105324	Acenaphthene-d10	15.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Vinyl benzoate	148	C9H8O2	000769-78-8	47
3			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47
4			2-(2-Oxo-2-phenyl-ethyl)-malon...	184	C11H8N2O	1000296-76-9	47
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47



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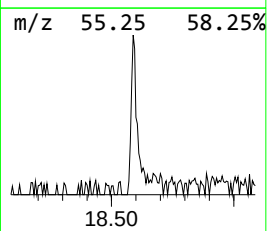
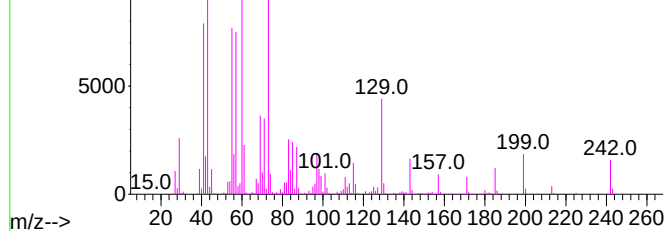
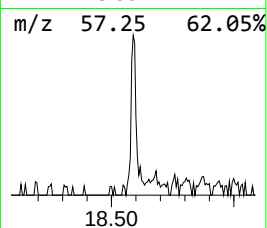
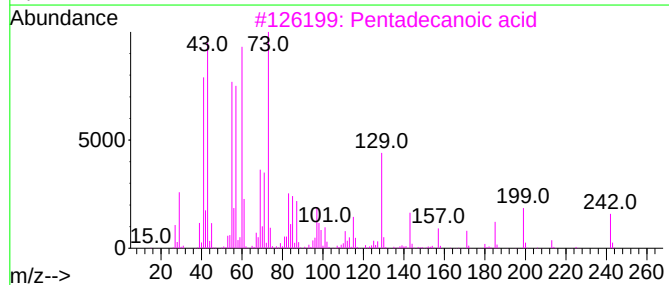
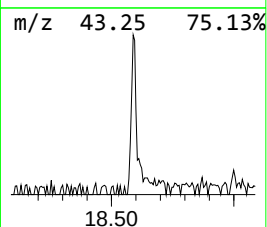
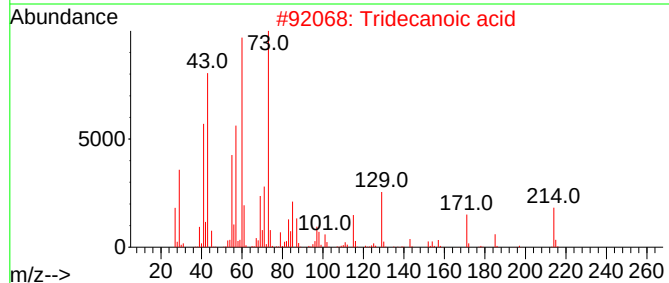
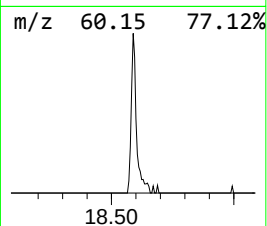
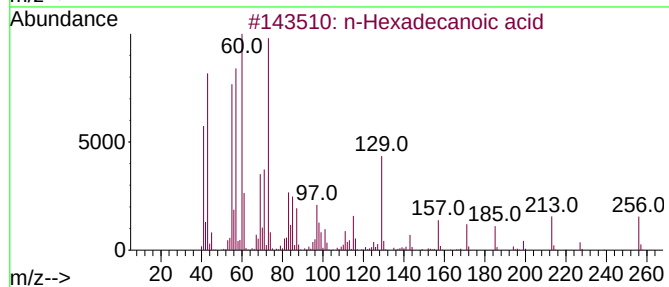
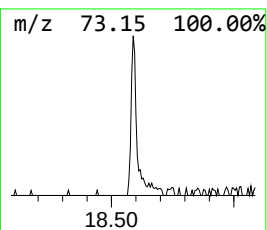
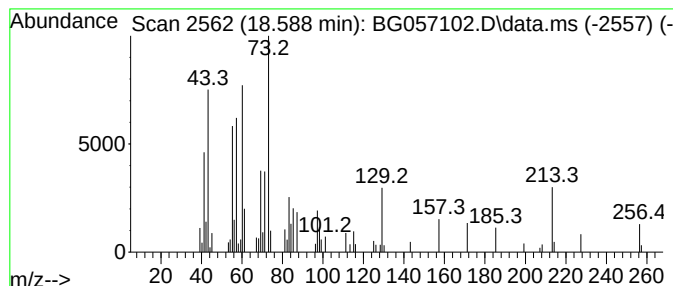
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.588	5.34 ng	69240	Phenanthrene-d10	17.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	52



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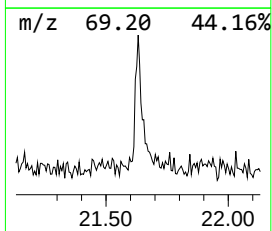
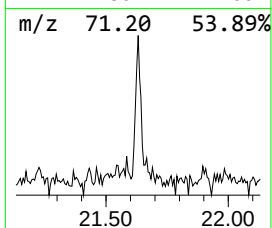
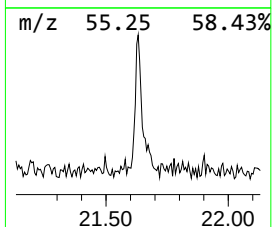
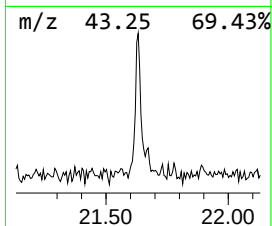
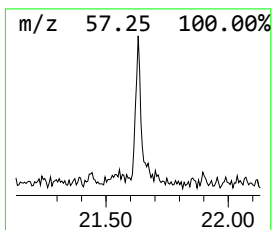
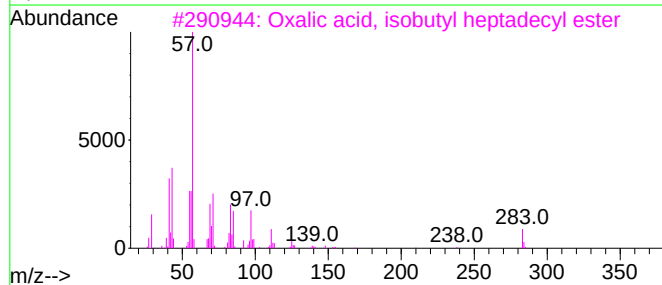
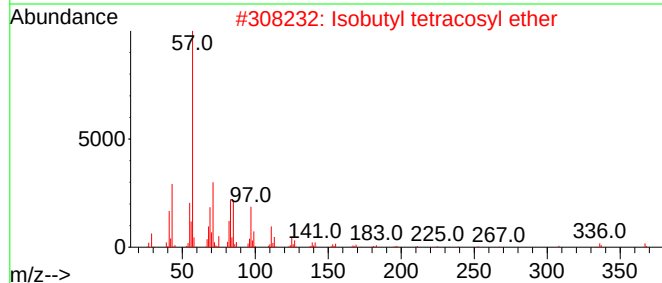
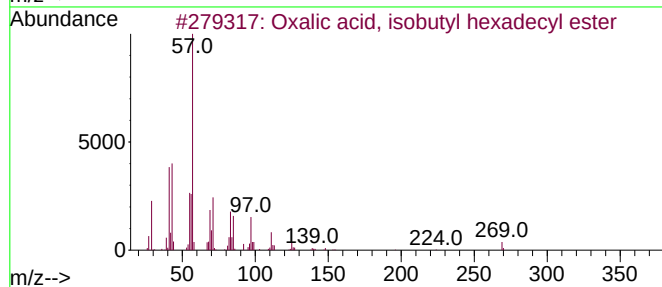
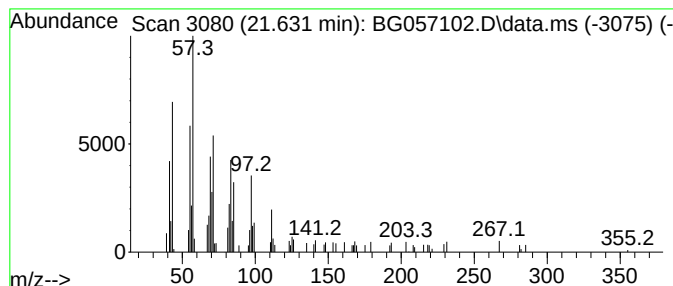
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Oxalic acid, isobutyl hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.631	4.68 ng	62267	Chrysene-d12	22.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2			Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	91
3			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87
4			1-Hexacosanol	382	C26H54O	000506-52-5	83
5			2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.436	24.4	ng	139843	1	8.402	114764	20.0
Benzophenone	16.350	9.6	ng	105324	3	15.017	219022	20.0
n-Hexadecanoic ...	18.588	5.3	ng	69240	4	17.754	259547	20.0
Oxalic acid, is...	21.631	4.7	ng	62267	5	22.072	266052	20.0